STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 177153

TO: Rei-Tsang Shiao **Location: rem/5A10/5C18** **Art Unit: 1626** **Tuesday, January 31, 2006** **Case Serial Number: 10/731108**	**From: Mary Hale** **Location: Biotech/Chem Library** **Rem 1D86** **Phone: 2-2507** **Mary.Hale@uspto.gov**

Search Notes

Feel free to contact me if you have any questions.

Note -- results are printed on both sides of printout

Shias
10/731108


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=> dis his

     (FILE 'HOME' ENTERED AT 16:10:59 ON 31 JAN 2006)

     FILE 'CASREACT' ENTERED AT 16:11:08 ON 31 JAN 2006
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L2              STR L1
L3            0 S L2
L4            2 S L2 FUL

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L2              STR
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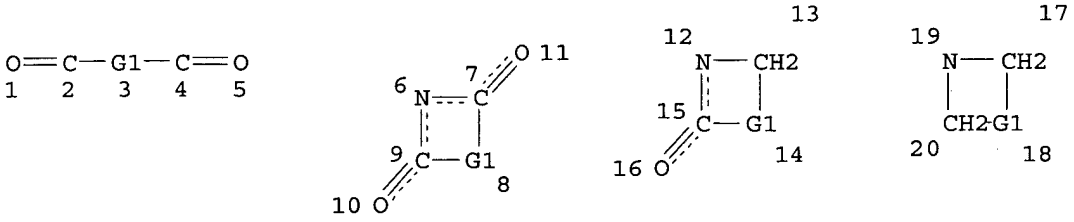


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  20

STEREO ATTRIBUTES: NONE


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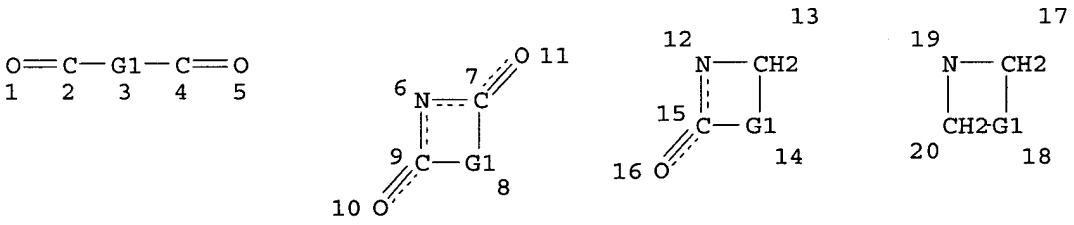


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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
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NUMBER OF NODES IS  20

STEREO ATTRIBUTES: NONE
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100.0% DONE    3276 VERIFIED       0 HIT RXNS                    0 DOCS
SEARCH TIME: 00.00.01


Prepared by: Mary Hale @2-2507 Rem Bldg 1D86
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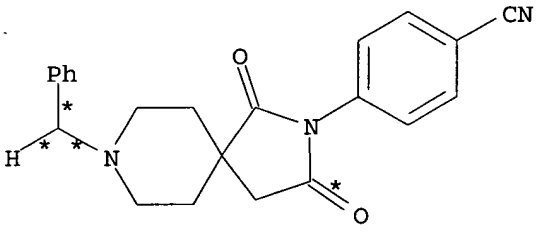
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 62097 TO 68943
PROJECTED ANSWERS: 0 TO 0

=> d l4 fhit ibib abs

L4 ANSWER 1 OF 2 CASREACT COPYRIGHT 2006 ACS on STN

RX(163) OF 590 COMPOSED OF RX(5), RX(6), RX(7), RX(14)
RX(163) 2 **O** + 2 X + **AR** ===> **AS**



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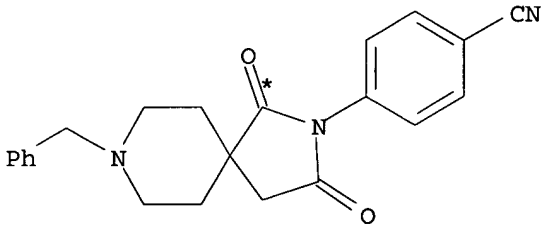

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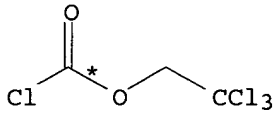
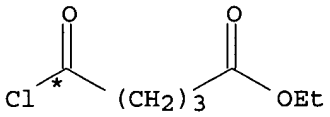
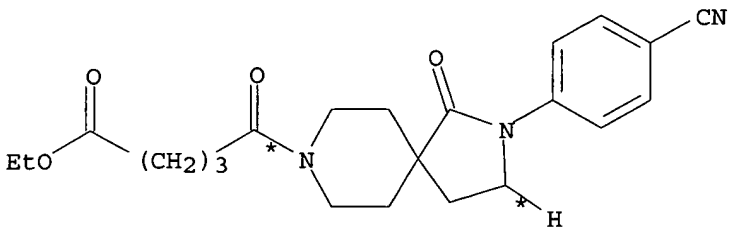


2 X



AR

4
STEPS



AS
YIELD 92%

RX(5) RCT O **685544-29-0**

STAGE(1)
RGT T 16940-66-2 NaBH4
SOL 67-56-1 MeOH
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) room temperature

STAGE(2)
RGT U 64-19-7 AcOH

STAGE(3)
RGT T 16940-66-2 NaBH4
SOL 76-05-1 F3CCO2H
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) room temperature

PRO R 685544-31-4, S 685544-30-3
NTE reaction is extremely vigorous in third stage

RX(6) RCT S 685544-30-3, R 685544-31-4, X 17341-93-4
PRO Y 685544-33-6, Z 685544-32-5
SOL 75-05-8 MeCN, 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) overnight, room temperature
NTE 85% overall yield, 8:2 mixture of starting lactams used

RX(7) RCT Z 685544-32-5
RGT AC 631-61-8 NH4OAc
PRO AB 685544-34-7
SOL 109-99-9 THF, 7732-18-5 Water
CON SUBSTAGE(1) room temperature, pH 5
SUBSTAGE(2) room temperature
NTE Cd-Pb couple used

RX(14) RCT AB 685544-34-7, AR **5205-39-0**
RGT AT 7087-68-5 EtN(Pr-i)2
PRO AS **685544-38-1**
SOL 68-12-2 DMF
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 4 hours, room temperature

ACCESSION NUMBER: 140:385509 CASREACT

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

TITLE: Discovery of Novel 2,8-Diazaspiro[4.5]decanes as Orally Active Glycoprotein IIb-IIIa Antagonists

AUTHOR(S): Mehrotra, Mukund M.; Heath, Julie A.; Smyth, Mark S.; Pandey, Anjali; Rose, Jack W.; Seroogy, Joseph M.; Volkots, Deborah L.; Nannizzi-Alaimo, Lisa; Park, Gary L.; Lambing, Joseph L.; Hollenbach, Stanley J.; Scarborough, Robert M.

CORPORATE SOURCE: Millennium Pharmaceuticals Inc., South San Francisco, CA, 94080, USA

SOURCE: Journal of Medicinal Chemistry (2004), 47(8), 2037-2061
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

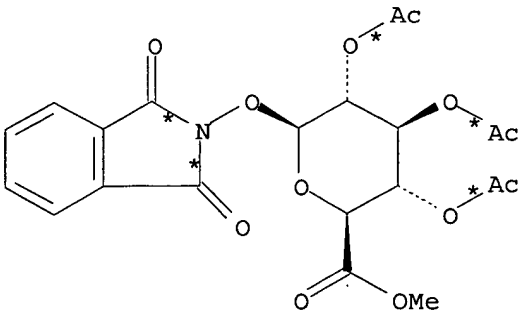
AB In our efforts to develop orally active GPIIb-IIIa antagonists with improved pharmaceutical properties, we have utilized a novel 2,8-diazaspiro[4.5]decane scaffold as a template. We describe here our investigation of a variety of templates including spiropiperidinyl-γ-lactams, spiropiperidinylimide, spiropiperidinylureas, and spiropiperidinylhydantoins. With the appropriate acidic and basic pharmacophores in place, each template yielded analogs with potent GPIIb-IIIa inhibitory activity. One of the compds., 59 (CT50787), was also used to demonstrate for the first time the use of a pharmacol. agent which is αIIbβ3 specific to display biol. activity in a lower species such as mouse and to extend bleeding times. Evaluation of the pharmacokinetic properties of selected compds. from each series in rat, dog, and cynomolgus monkey has led to the identification of 22 (CT51464), a double prodrug, with excellent pharmacokinetic properties. It exhibited good pharmacokinetic profile across species (F% = 33 (Cyno), 73 (dog), 22 (rat); t1/2β = 14.2 h (Cyno), 8.97 h (dog), 1.81 h (rat)). The biol. active form, 23 (CT50728), displayed inhibition of platelet aggregation in platelet rich plasma (PRP) with an IC50 value of 53 nM in citrate buffer, 110 nM in PPACK anticoagulated PRP, and 4 nM in solid-phase GPIIb-IIIa competition binding assay (ELISA). Both 23 and 22 were stable in human liver microsomes, did not inhibit the P 450 3A4 isoenzyme, and had low protein binding (18.22% for 23) and a desirable log P (0.45±0.06 for 22, and -0.91±0.32 for 23). It is predicted that the high oral bioavailability for these compds. in multiple species should translate into lower intra- and intersubject variability in man. The long plasma half-life of the lead is consistent with once or twice daily administration for chronic therapy. Analog 22 (CT51464) thus appears to be a promising oral GPIIb-IIIa inhibitor with significantly improved pharmacokinetic properties over the previously described clin. candidates and may be found useful in the treatment of arterial occlusive disorders.

REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

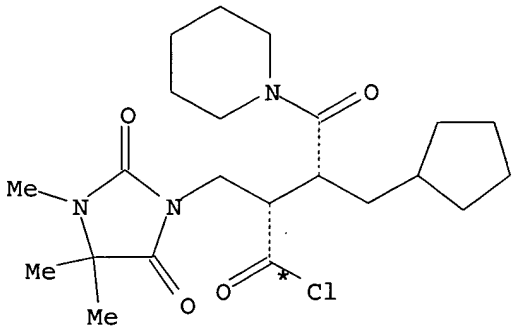
=> d l4 fhit ibib abs 2

L4 ANSWER 2 OF 2 CASREACT COPYRIGHT 2006 ACS on STN

RX(35) OF 82 COMPOSED OF RX(4), RX(6), RX(7), RX(10)
RX(35) **K** + **R** ===> AD

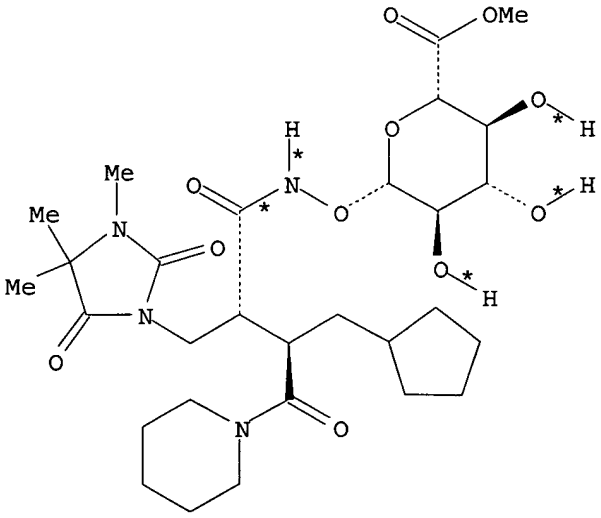


K



R

4
STEPS



AD
YIELD 92%

RX(4) RCT K **319926-19-7**
RGT P 302-01-2 N2H4
PRO O 319926-20-0
SOL 67-56-1 MeOH
NTE STEREOSELECTIVE

RX(6) RCT R **319926-22-2**, O 319926-20-0
RGT W 121-44-8 Et3N
PRO V 319926-23-3
SOL 75-09-2 CH2Cl2
NTE STEREOSELECTIVE

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

RX(7) RCT V 319926-23-3

STAGE(1)
RGT E 124-41-4 NaOMe
SOL 67-56-1 MeOH

STAGE(2)

PRO X 319926-24-4
NTE DUOLITE RESIN (H+FORM) USED IN SECOND STAGE , STEREOSELECTIVE

RX(10) RCT X 319926-24-4

STAGE(1)
RGT AE 25952-53-8 EDAP, AF 2592-95-2 1-Benzotriazolol, AG **872-50-4** NMEP, Q 174265-77-1 1-Piperidinebutanoic acid, β-(cyclopentylmethyl)-γ-oxo-α-[(3,4,4-trimethyl-2,5-dioxo-1-imidazolidinyl)methyl]-, (αR,βR)-
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT E 124-41-4 NaOMe
SOL 67-56-1 MeOH

STAGE(3)

PRO AD 319926-26-6
NTE DUOLITE RESIN (H+FORM) USED IN LAST STAGE , STEREOSELECTIVE

ACCESSION NUMBER: 134:116168 CASREACT
TITLE: The synthesis of the glucuronide adduct of Trocade
AUTHOR(S): Mitchell, Mark B.; Whitcombe, Ian W. A.
CORPORATE SOURCE: Chemical Synthesis Department, Roche Discovery Welwyn, Welwyn Garden City, AL7 3AY, UK
SOURCE: Tetrahedron Letters (2000), 41(45), 8829-8834
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthetic preparation of the glucuronide adduct of Trocade, a selective inhibitor of the MMP collagenase, is described. This was achieved by preparation of the protected O-glucuronsyl hydroxylamine and subsequent coupling to the available carboxylic acid, followed by deprotection. The synthetic material was identical to authentic isolated metabolite, which confirmed that glucuronidation of Trocade occurs on the oxygen of the hydroxamic acid.
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s werpy ?/au
L5 6 WERPY ?/AU

=> d 1-6 ibib abs

L5 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 141:123556 CASREACT
TITLE: Process for producing N-methylsuccinimide from dicarbonyl compounds by cyclization and alkylation and

hydrogenation to N-methylpyrrolidinone

INVENTOR(S): **Werpy, Todd A.**; Frye, John G., Jr.; White, James F.; Holladay, Johnathan E.; Zacher, Alan H.

PATENT ASSIGNEE(S): Battelle Memorial Institute, USA

SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2

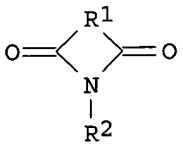
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004058708	A1	20040715	WO 2003-US40106	20031216
WO 2004058708	B1	20040923		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004176589	A1	20040909	US 2003-731108	20031210
EP 1572644	A1	20050914	EP 2003-814062	20031216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.: US 2002-435469P 20021220
US 2003-108336 20031210
US 2003-731108 20031210
WO 2003-US40106 20031216

OTHER SOURCE(S): MARPAT 141:123556

GI



I

AB The invention includes methods of processing an initial di-carbonyl compound by conversion to a cyclic compound I (R1 = linear or branched, saturated or unsatd. hydrocarbon or substituted hydrocarbon; R2 = H; linear, cyclic or branched, saturated or unsatd. alkyl; aromatic group). The cyclic compound is reacted with an alkylating agent to form a derivative having an alkylated ring nitrogen. The invention encompasses a method of producing an N-alkyl product. Ammonia content of a solution is adjusted to produce a ratio of ammonia to dicarboxylate compound of from about 1:1 to about 1.5:1. An alkylating agent is added and the initial compound is alkylated and cyclized. The invention includes methods of making N-methylpyrrolidinone (NMP). Aqueous ammonia and succinate is introduced into a vessel and ammonia is adjusted to provide a ratio of ammonia to succinate of less than 2:1. A methylating agent is reacted with succinate at a temperature of from greater

than 100° to about 400° to produce N-methylsuccinimide which is purified and hydrogenated to form NMP.

L5 ANSWER 2 OF 6 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 141:25334 CASREACT
TITLE: Methods of forming alpha, beta-unsaturated acids and esters
INVENTOR(S): Lilga, Michael A.; **Werpy, Todd A.**; Holladay, Johnathan E.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 9 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004110974	A1	20040610	US 2002-315404	20021209
PRIORITY APPLN. INFO.:			US 2002-315404	20021209

OTHER SOURCE(S): MARPAT 141:25334
AB In the method, a carboxylic acid is mixed with an α-hydroxy acid or an α-hydroxy ester and is esterified to form an α-acyloxy derivative The α-acyloxy derivative is transformed into an α,β-unsatd. derivative The invention addnl. includes a process of forming an acrylate. Lactic acid or a lactic acid ester is reacted with a first portion of acetic acid in the presence of a first catalyst to produce the corresponding 2-acetoxy propionic acid or ester. A non-reacted portion of the acetic acid is recycled. The 2-acetoxypropionic acid or ester is transferred to a second vessel containing a second catalyst, and acetic acid is liberated from the 2-acetoxypropionic acid or ester to produce a corresponding acrylic acid or acrylate ester. The acid or ester is subsequently esterified by reaction with an alc. to form a desired acrylate ester.

L5 ANSWER 3 OF 6 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 138:339970 CASREACT
TITLE: Hydrogenolysis of 6-carbon sugars and other organic compounds using multimetallic catalysts
INVENTOR(S): **Werpy, Todd A.**; Frye, John G., Jr.; Zacher, Alan H.; Miller, Dennis J.
PATENT ASSIGNEE(S): Battelle Memorial Institute, USA; Michigan State University
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003035582	A1	20030501	WO 2002-US33982	20021023
WO 2003035582	B1	20031211		

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LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003119952	A1	20030626	US 2001-836	20011023
US 6841085	B2	20050111		
EP 1440046	A1	20040728	EP 2002-784244	20021023

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

PRIORITY APPLN. INFO.:	US 2001-836	20011023
	WO 2002-US33982	20021023

AB Methods for hydrogenolysis are described which use a Re-containing multimetallic catalyst for hydrogenolysis of both C-O and C-C bonds. Methods and compns. for reactions of hydrogen over a Re-containing catalyst with compns. containing a 6-carbon sugar, sugar alc., or glycerol are described. It has been surprisingly discovered that reaction with hydrogen over a Re-containing multimetallic catalyst resulted in superior conversion and selectivity to desired products such as propylene glycol.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 6 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	137:325152 CASREACT
TITLE:	Hydrogenolysis of 5-carbon sugars, sugar alcohols, and other methods and compositions for reactions involving hydrogen
INVENTOR(S):	**Werpy, Todd A.**; Frye, John G., Jr.; Zacher, Alan H.; Miller, Dennis J.
PATENT ASSIGNEE(S):	Battelle Memorial Institute, USA
SOURCE:	U.S., 18 pp. CODEN: USXXAM
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6479713	B1	20021112	US 2001-12890	20011023
US 2003130545	A1	20030710	US 2002-214983	20020806
US 6677385	B2	20040113		
WO 2003035593	A1	20030501	WO 2002-US33983	20021023
WO 2003035593	B1	20031113		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1440048	A1	20040728	EP 2002-786487	20021023

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

US 2004064003 A1 20040401 US 2003-676497 20030930
PRIORITY APPLN. INFO.: US 2001-12890 20011023
US 2002-214983 20020806
WO 2002-US33983 20021023

AB Methods and compns. for reactions of hydrogen over a Re-containing catalyst with compns. containing a 5-carbon sugar, sugar alc., or lactic acid are described. It has been surprisingly discovered that reaction with hydrogen over a Re-containing multimetallic catalyst resulted in superior conversion and selectivity to desired products such as propylene glycol (PG). A process for the synthesis of PG from lactate or lactic acid is also described.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 6 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 137:5076 CASREACT
TITLE: Biorefinery concept development based on wheat flour milling
AUTHOR(S): Elliott, Douglas C.; Orth, Rick J.; Gao, Johnway; **Werpy, Todd A.**; Eakin, David E.; Schmidt, Andrew J.; Neuenschwander, Gary G.; Flagg, Anthony J.; Murry, Jim; Lahman, Lyle; Lin, C. J.; Mennel, Donald L.; Landucci, Ron
CORPORATE SOURCE: Pacific Northwest National Laboratory, Richland, WA, 99352, USA
SOURCE: Preprints of Symposia - American Chemical Society, Division of Fuel Chemistry (2002), 47(1), 361-362
CODEN: PSADFZ; ISSN: 1521-4648
PUBLISHER: American Chemical Society, Division of Fuel Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An overview describing the production of polyols or lactic acid using a wheat millfeed as a source of raw starch. Starch was extract from wheat millfeed using hot water followed by filtration to remove the fibrous material contained in the extract The fibrous material was found to be useful as an animal feed byproduct. The raw starch was then enzymically liquefied and saccharified to produce dextrose. The dextrose then served as a substrate for fermentation to produce lactic acid or for catalytic hydrogenation to produce sorbitol.

L5 ANSWER 6 OF 6 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 136:340398 CASREACT
TITLE: Alpha-ester compounds and their thermal decomposition into acrylates and lactones or anhydrides
INVENTOR(S): **Werpy, Todd A.**; Lilga, Michael A.
PATENT ASSIGNEE(S): Battelle Memorial Institute, USA
SOURCE: PCT Int. Appl., 15 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002032849	A2	20020425	WO 2001-US31570	20011009
WO 2002032849	A3	20020718		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ,
VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 6545175	B1	20030408	US 2000-691143	20001019
AU 2002013078	A5	20020429	AU 2002-13078	20011009
EP 1328502	A2	20030723	EP 2001-981437	20011009
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CN 1529690	A	20040915	CN 2001-820734	20011009
BR 2001014593	A	20050111	BR 2001-14593	20011009
PRIORITY APPLN. INFO.:			US 2000-691143	20001019
			WO 2001-US31570	20011009

OTHER SOURCE(S): MARPAT 136:340398

AB Alpha-ester compds. R3O2CC(R2)[O2CC(R9)(R8)(CR7R6)nC(R4)(R3)CO2R1]C(R10)(R11)(R12) [n = 0, 1; R2-R12 = H, C1-10 alkyl(oxy), C6-10 aryl(oxy), aralkyl; R1 = H, C1-10 alkyl, C6-10 aryl, aralkyl], which decompose at >200° to an acrylate and a lactone or anhydride (no data; where the lactone or anhydride has a b.p. of <170°/1 atmospheric), are prepared Thus, Me lactate and succinic anhydride were heated to 70° in the presence of sulfuric acid, methanol and chloroform added, and the mixt refluxed to give Me 1-(methoxycarbonyl)ethyl succinate in 98.5% yield.

=> => dis his

(FILE 'HOME' ENTERED AT 16:10:59 ON 31 JAN 2006)

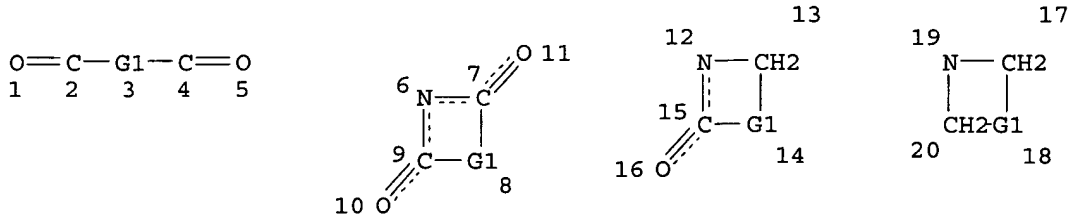
FILE 'CASREACT' ENTERED AT 16:11:08 ON 31 JAN 2006

L1		STR
L2		STR L1
L3	0	S L2
L4	2	S L2 FUL
L5	6	S WERPY ?/AU

FILE 'CASREACT' ENTERED AT 16:20:25 ON 31 JAN 2006

L6		STR L3
L7	50	S L6
L8	2816	S L6 FUL
L9		STR L2
L10	9	SEARCH L9 SUB=L8 FUL
L11	7	S L10 NOT L4

=> d l11 que stat
L2 STR



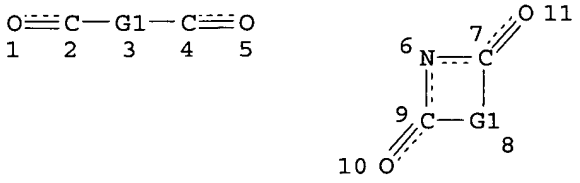
REP G1=(2-4) C

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

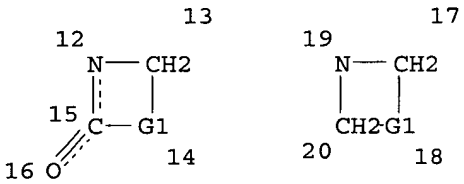
STEREO ATTRIBUTES: NONE
L4 2 SEA FILE=CASREACT SSS FUL L2 (42 REACTIONS)
L6 STR



REP G1=(2-4) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L8 2816 SEA FILE=CASREACT SSS FUL L6 (52585 REACTIONS)
L9 STR



REP G1=(2-4) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L10 9 SEA FILE=CASREACT SUB=L8 SSS FUL L9 (124 REACTIONS)
L11 7 SEA FILE=CASREACT ABB=ON PLU=ON L10 NOT L4

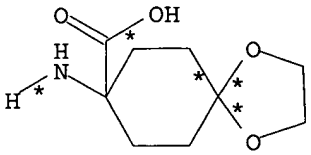
=> d 1-7 fhit ibib abs

L11 ANSWER 1 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

RX(21) OF 22 COMPOSED OF RX(8), RX(9), RX(5)

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

RX(21) AT + AL + AD + C + AE ===> AF



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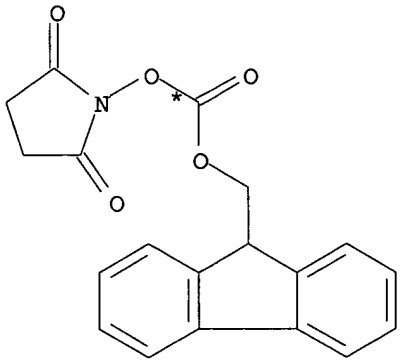
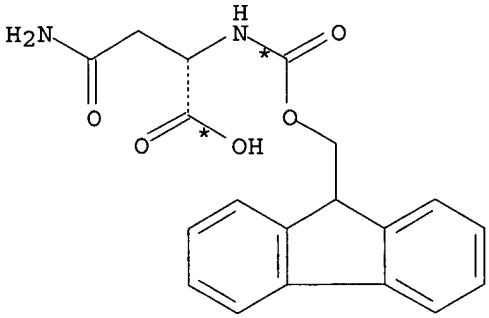
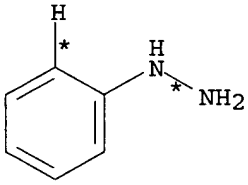


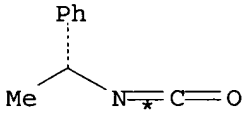
AL



AD

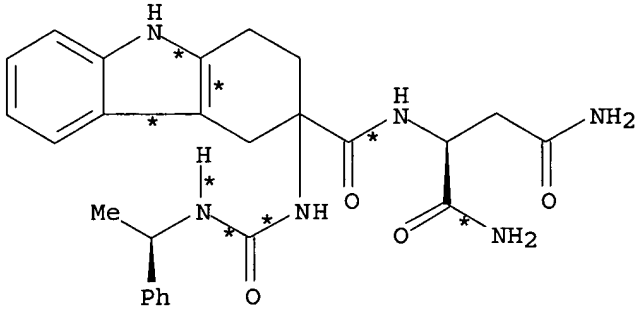


C



AE

3
STEPS



AF

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

RX(8) RCT AT 54621-18-0, AL 82911-69-1

STAGE(1)
RGT AP 121-44-8 Et3N, AO 1310-73-2 NaOH
SOL 7732-18-5 Water, 75-05-8 MeCN
CON overnight, room temperature, pH 9

STAGE(2)
RGT AR 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, acidify

PRO AU 369403-24-7

RX(9) RCT AU 369403-24-7
RGT AR 7647-01-0 HCl
PRO B 285996-74-9
SOL 7732-18-5 Water, 67-64-1 Me2CO
CON 4 hours, room temperature

RX(5) RCT AD 71989-16-7

STAGE(1)
RGT G 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium, 1-[bis(dimethylamino)methylene]-, hexafluorophosphate(1-), 3-oxide, H 109-02-4 N-Methylmorpholine
SOL 68-12-2 DMF

STAGE(2)
RGT I **110-89-4** Piperidine
SOL 68-12-2 DMF

STAGE(3)
RCT B 285996-74-9
RGT G 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium, 1-[bis(dimethylamino)methylene]-, hexafluorophosphate(1-), 3-oxide, H 109-02-4 N-Methylmorpholine
CAT 1122-58-3 4-DMAP
SOL 68-12-2 DMF

STAGE(4)
RCT C 100-63-0
RGT J 64-19-7 AcOH, K 7646-85-7 ZnCl2, L **872-50-4** NMEP
CON 20 hours, 70 deg C

STAGE(5)
RGT I **110-89-4** Piperidine
SOL 68-12-2 DMF

STAGE(6)
RCT AE 33375-06-3
SOL 107-06-2 ClCH2CH2Cl
CON 18 hours, room temperature

STAGE(7)
RGT O 76-05-1 F3CCO2H

PRO AF 846567-74-6
NTE reactant bound onto resin

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

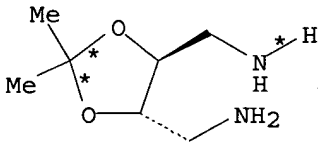
ACCESSION NUMBER: 142:261363 CASREACT
TITLE: Solid-phase synthesis of substituted 3-amino-3'-carboxytetrahydrocarbazoles
AUTHOR(S): Koppitz, Marcus; Reinhardt, Gabriele; van Lingen, Anneke
CORPORATE SOURCE: Automated Medicinal Chemistry, Schering AG, Berlin, 13342, Germany
SOURCE: Tetrahedron Letters (2005), 46(6), 911-914
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two related solid-phase synthesis routes have been developed allowing the synthesis of 3-amino-3'-carboxy substituted tetrahydrocarbazole derivs. Diversity can be introduced at the amino and carboxy functionalities and at the nitrogen and the aromatic ring of the tetrahydrocarbazole moiety. Both routes rely on Fmoc-protected 1-amino-4-oxocyclohexanecarboxylic acid as central core element. Derivatization of the carboxy function is achieved with amines; derivatization of the amino functionality is possible by reaction with alkyl halides, isocyanates, activated alcs., sulfonic acid chlorides or carboxylic acids. The tetrahydrocarbazole scaffold is generated by Fischer indole cyclization with phenylhydrazine derivs., thereby introducing diversity in the aromatic moiety. N-Alkylation at the indole nitrogen with alkyl halides delivers N-substituted derivs.

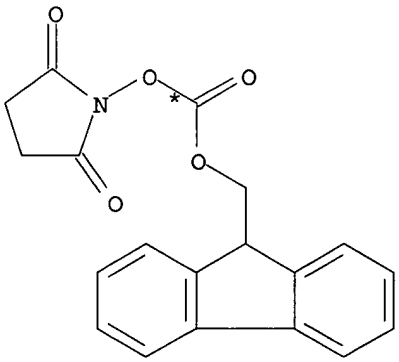
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

RX(80) OF 248 COMPOSED OF RX(15), RX(17), RX(24)
RX(80) AR + AN + AV + BT ===> BZ



AR



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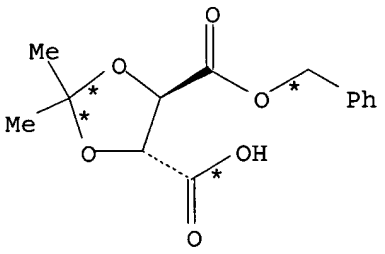


AV

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

3
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(15) RCT AR 119322-88-2, AN 82911-69-1
RGT AP 121-44-8 Et3N
PRO AS 675606-43-6
SOL 109-99-9 THF
CON 30 minutes, 0 deg C

RX(17) RCT AS 675606-43-6, AV 197457-57-1
RGT BA **132705-51-2** Phosphorus(1+), bromotri-1-pyrrolidinyl-, (T-4)-, hexafluorophosphate(1-), BB 7087-68-5 EtN(Pr-i)2
PRO AZ 675606-44-7
SOL 68-12-2 DMF
CON 17 hours, room temperature

RX(24) RCT AZ 675606-44-7

STAGE(1)
RGT BA **132705-51-2** Phosphorus(1+), bromotri-1-pyrrolidinyl-, (T-4)-, hexafluorophosphate(1-), BB 7087-68-5 EtN(Pr-i)2, BV **872-50-4** NMEP
SOL 75-09-2 CH2Cl2
CON 4 hours, room temperature

STAGE(2)
RGT BW 108-24-7 Ac2O, BV **872-50-4** NMEP
SOL 75-09-2 CH2Cl2
CON 3 hours, room temperature

STAGE(3)
RGT BX 110-89-4 Piperidine
SOL 75-09-2 CH2Cl2, 68-12-2 DMF
CON 3 hours, room temperature

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

STAGE(4)
RCT BT 635287-20-6
RGT BY 2592-95-2 1-Benzotriazolol, BI 25952-53-8 EDAP
SOL 68-12-2 DMF
CON 6 hours, room temperature

STAGE(5)
RGT BW 108-24-7 Ac2O
SOL 68-12-2 DMF
CON 1 hour, room temperature

PRO BZ 758718-14-8D
NTE solid-supported reaction, attachment of spacer (first two stages) repeated up to three times, first stage attachment to TOYOPEARL or AffiGel resin

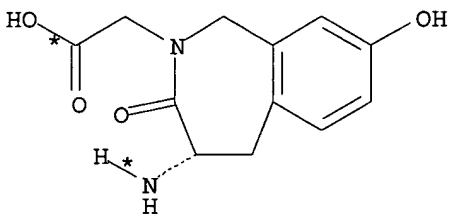
ACCESSION NUMBER: 141:273853 CASREACT
TITLE: Design and synthesis of novel hydrophilic spacers for the reduction of nonspecific binding proteins on affinity resins
AUTHOR(S): Shiyama, Takaaki; Furuya, Minoru; Yamazaki, Akira; Terada, Tomohiro; Tanaka, Akito
CORPORATE SOURCE: Chemistry Department, Reverse Proteomics Research Institute Co., Ltd, Chiba, 292-0818, Japan
SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(11), 2831-2841
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Tubulin and actin often bind nonspecifically to affinity chromatog. resins, complicating research toward identifying the cellular targets. Reduction of nonspecific binding proteins is important for success in finding such targets. We herein disclose the design, synthesis, and effectiveness in reduction of nonspecific binding proteins, of novel hydrophilic spacers (2-5), which were introduced between matrixes and a ligand. Among them, tartaric acid derivative (5) exhibited the most effective reduction of nonspecific binding proteins, while maintaining binding of the target protein. Introduction of 5 on TOYOPEARL reduced tubulin and actin by almost 65% and 90% compared to that without the hydrophilic spacer, resp., with effective binding to the target protein, FKBP12.

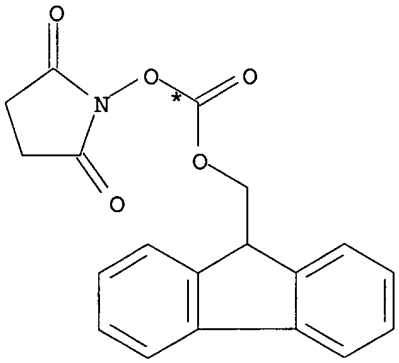
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

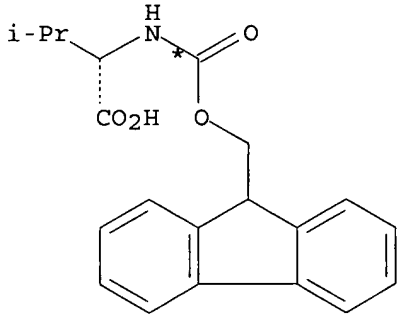
RX(14) OF 31 COMPOSED OF RX(8), RX(4)
RX(14) **AC** + AF + A + 4 B + 2 D ===> T



AC



AF



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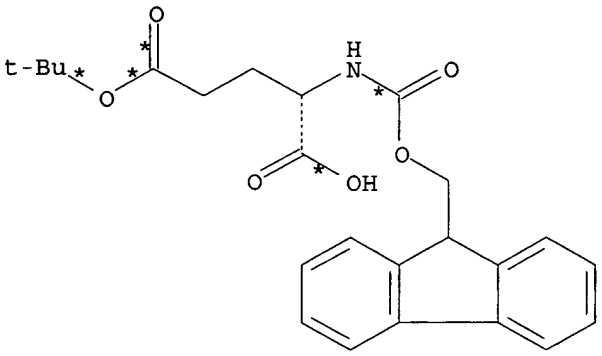
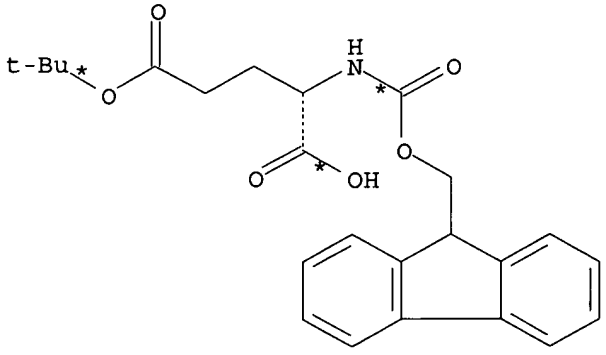
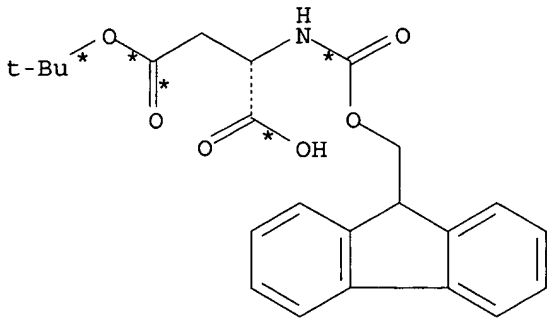


B



3 B

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

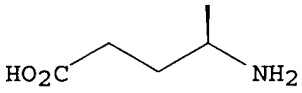


2 D

2 STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



T

RX(8) RCT AC **446255-98-7**, AF 82911-69-1
RGT AG 497-19-8 Na2CO3
PRO S 446255-99-8
SOL 7732-18-5 Water, 123-91-1 Dioxane
CON overnight, room temperature

RX(4) RCT A 68858-20-8

STAGE(1)
SOL 68-12-2 DMF

STAGE(2)
RGT F **110-89-4** Piperidine
CON 24 minutes, room temperature

STAGE(3)
RCT B 71989-18-9
RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF

STAGE(4)
RGT F **110-89-4** Piperidine
CON 24 minutes, room temperature

STAGE(5)
RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF

STAGE(6)
RGT F **110-89-4** Piperidine
CON 24 minutes, room temperature

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

STAGE(7)
RCT S 446255-99-8
RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF

STAGE(8)
RGT F **110-89-4** Piperidine
CON 24 minutes, room temperature

STAGE(9)
RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF

STAGE(10)
RGT F **110-89-4** Piperidine
CON 24 minutes, room temperature

STAGE(11)
RCT D 71989-14-5
RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF

STAGE(12)
RGT F **110-89-4** Piperidine
CON 24 minutes, room temperature

STAGE(13)
RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF

STAGE(14)
RGT F **110-89-4** Piperidine
CON 24 minutes, room temperature

STAGE(15)
RGT G 94790-37-1 HBTU, H 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF

STAGE(16)
RGT F **110-89-4** Piperidine
CON 24 minutes, room temperature

STAGE(17)
RGT I 6485-79-6 Silane, tris(1-methylethyl)-, J 7732-18-5 Water, K 76-05-1 F3CCO2H, L 100-66-3 PhOMe

PRO T 446256-02-6
NTE solid-supported reaction, attachment to Wang resin in first stage, reactants assumed in seventh, eleventh, thirteenth stages

ACCESSION NUMBER: 140:107390 CASREACT
TITLE: Conformational constraints of tyrosine in protein tyrosine kinase substrates: Information about preferred bioactive side-chain orientation
AUTHOR(S): Ruzza, Paolo; Calderan, Andrea; Donella-Deana, Arianna; Biondi, Barbara; Cesaro, Luca; Osler, Alessio; Elardo, Stefano; Guiotto, Andrea; Pinna, Lorenzo A.; Borin, Gianfranco
CORPORATE SOURCE: Padova Unit, CNR, Institute of Biomolecular Chemistry, Padua, 35131, Italy

SOURCE: Biopolymers (2003), 71(4), 478-488
CODEN: BIPMAA; ISSN: 0006-3525
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

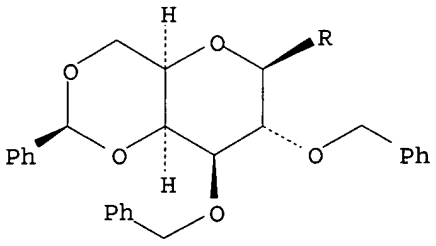
AB The side-chain orientation of a tyrosine residue located in a peptide, which is an excellent substrate of Syk tyrosine kinase, was fixed in the gauche (+) or gauche (-) conformation by using the 7-hydroxy-1,2,3,4-tetrahydro isoquinoline-3-carboxylic (Htc) structure. The tyrosine trans conformation was blocked by using an aminobenzazepine-type (Hba) structure. The proposed side-chain orientations were confirmed by the anal. of the 1H-NMR parameters: chemical shifts, coupling consts., and nuclear Overhauser effects to the tyrosine constraints in the different analogs. This "rotamer scan" of the phosphorylatable residue allowed us to generate optimal substrates in terms of both phosphorylation efficiency and selectivity for Syk tyrosine kinase. In contrast, these conformationally restricted tyrosine analogs were not tolerated by the Src-related tyrosine kinases Lyn and c-Fgr.

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

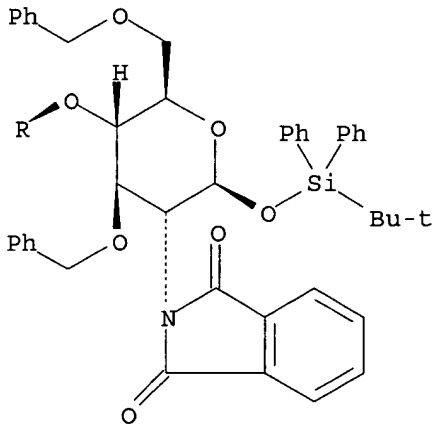
L11 ANSWER 4 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

RX(125) OF 275 COMPOSED OF RX(10), RX(11), RX(12), RX(2), RX(23), RX(24), RX(25), RX(16)
RX(125) AF + AK + BZ + 2 AS + BA + BB + BC + BD + BE + BF ===> BG

PAGE 1-A



PAGE 2-A



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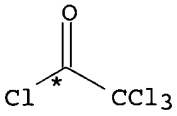

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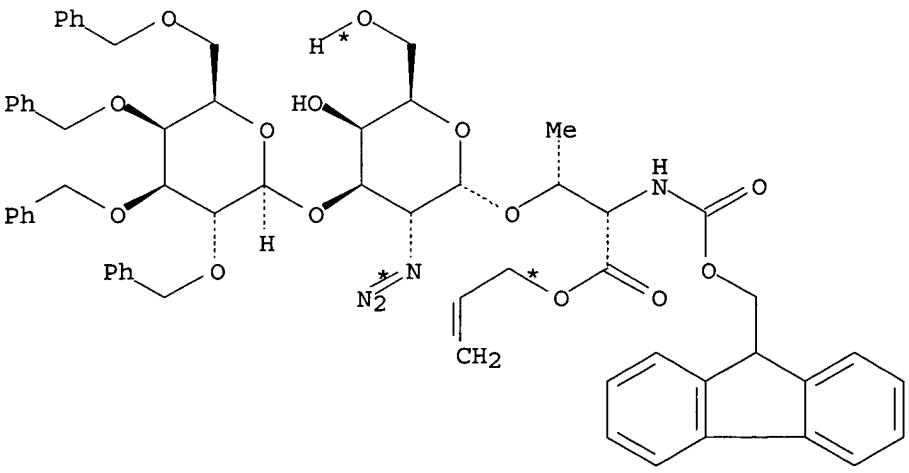
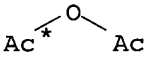
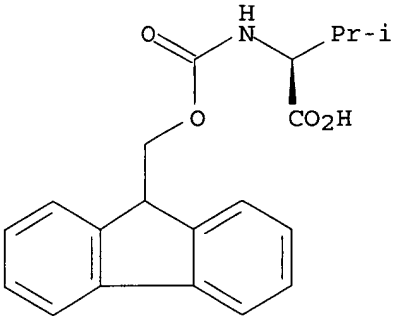


BZ



2 AS

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86



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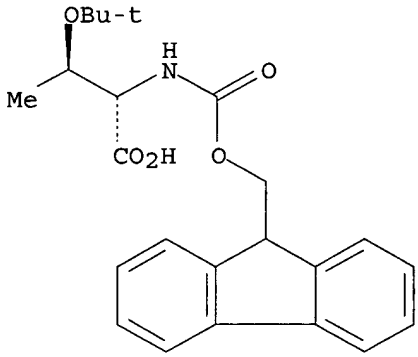

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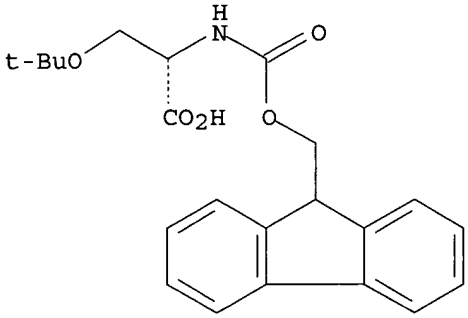

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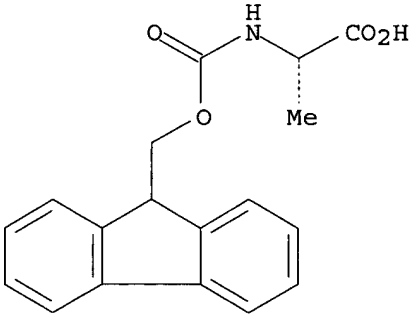

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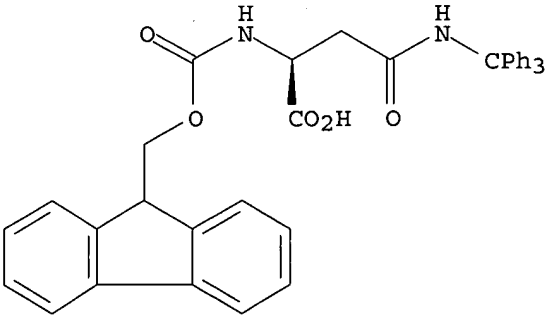

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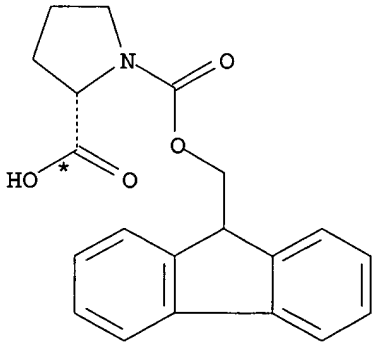


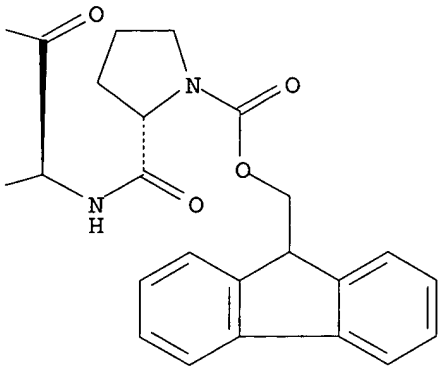
BF

8
STEPS

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 1-B



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(10) RCT AF 503830-97-5
RGT AI 107-15-3 H2NCH2CH2NH2
PRO AH 503830-98-6
SOL 71-36-3 BuOH
CON 18 hours, 95 deg C
NTE alternative prepn. shown

RX(11) RCT AH 503830-98-6, AK 76-02-8
RGT AM 110-86-1 Pyridine
PRO AL 503830-99-7
CON overnight, 0 deg C

RX(12) RCT AL 503830-99-7
RGT AN 429-41-4 Bu4N.F
PRO E 620964-97-8
SOL 109-99-9 THF, 64-19-7 AcOH
CON overnight, room temperature
NTE stereoselective

RX(2) RCT E 620964-97-8

STAGE(1)
RGT G 38078-09-0 DAST [(Et2N).SF3]
SOL 109-99-9 THF
CON 30 minutes, 0 deg C

STAGE(2)
RGT H 67-56-1 MeOH

PRO F 503831-01-4
NTE stereoselective

RX(23) RCT BZ 503830-92-0

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STAGE(1)
RGT AQ 1291-32-3 ZrCp2Cl2, AR 7783-93-9 AgClO4
SOL 75-09-2 CH2Cl2
CON 1 hour, -15 deg C

STAGE(2)
RCT F 503831-01-4
SOL 75-09-2 CH2Cl2
CON 2.5 hours, room temperature

STAGE(3)
RGT L 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CA 503831-03-6

RX(24) RCT CA 503831-03-6

STAGE(1)
RGT AT 7440-66-6 Zn, AO 64-19-7 AcOH
SOL 75-09-2 CH2Cl2
CON 72 hours, room temperature

STAGE(2)
RCT AS 108-24-7
SOL 67-56-1 MeOH, 75-09-2 CH2Cl2
CON 40 minutes, room temperature

PRO CB 503831-05-8

RX(25) RCT CB 503831-05-8
PRO AU 503831-07-0
CAT 14221-01-3 Pd(PPh3)4
SOL 109-99-9 THF
CON overnight, room temperature

RX(16) RCT BA 68858-20-8

STAGE(1)
RGT BH 538-75-0 DCC, BI 2592-95-2 1-Benzotriazolol
SOL 872-50-4 NMEP
CON 1 hour, room temperature

STAGE(2)
RGT BJ 7087-68-5 EtN(Pr-i)2, BK **872-50-4** NMEP
SOL 108-24-7 Ac2O

STAGE(3)
RCT BB 71989-35-0
RGT BH 538-75-0 DCC, BI 2592-95-2 1-Benzotriazolol
SOL 872-50-4 NMEP
CON 1 hour, room temperature

STAGE(4)
RGT BJ 7087-68-5 EtN(Pr-i)2, BK **872-50-4** NMEP
SOL 108-24-7 Ac2O

STAGE(5)
RCT BC 71989-33-8

RGT BH 538-75-0 DCC, BI 2592-95-2 1-Benzotriazolol
SOL 872-50-4 NMEP
CON 1 hour, room temperature

STAGE(6)
RGT BJ 7087-68-5 EtN(Pr-i)2, BK **872-50-4** NMEP
SOL 108-24-7 Ac2O

STAGE(7)
RCT BD 35661-39-3
RGT BH 538-75-0 DCC, BI 2592-95-2 1-Benzotriazolol
SOL 872-50-4 NMEP
CON 1 hour, room temperature

STAGE(8)
RGT BJ 7087-68-5 EtN(Pr-i)2, BK **872-50-4** NMEP
SOL 108-24-7 Ac2O

STAGE(9)

STAGE(10)
RCT BE 132388-59-1
RGT BH 538-75-0 DCC, BI 2592-95-2 1-Benzotriazolol
SOL 872-50-4 NMEP
CON 1 hour, room temperature

STAGE(11)
RGT BJ 7087-68-5 EtN(Pr-i)2, BK **872-50-4** NMEP
SOL 108-24-7 Ac2O

STAGE(12)
RGT BL **110-89-4** Piperidine
SOL 872-50-4 NMEP
CON 5 minutes, room temperature

STAGE(13)
RCT AU 503831-07-0
RGT BM 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium,
1-[bis(dimethylamino)methylene]-, hexafluorophosphate(1-),
3-oxide, BJ 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP

STAGE(14)
RCT BF 71989-31-6
RGT BH 538-75-0 DCC, BI 2592-95-2 1-Benzotriazolol
SOL 872-50-4 NMEP
CON 1 hour, room temperature

STAGE(15)
RGT BJ 7087-68-5 EtN(Pr-i)2, BK **872-50-4** NMEP
SOL 108-24-7 Ac2O

STAGE(16)
RGT K 76-05-1 F3CCO2H
SOL 75-18-3 Me2S, 108-39-4 3-Methylphenol, 540-63-6 HSCH2CH2SH
CON room temperature -> -15 deg C

STAGE(17)
RGT AW 1493-13-6 F3CSO2H
CON 1 hour, -15 deg C

STAGE(18)
RGT AM 110-86-1 Pyridine
SOL 60-29-7 Et2O

PRO BG 503831-12-7
NTE solid-supported reaction, Sieber amide resin used, alternative cleavage step showed

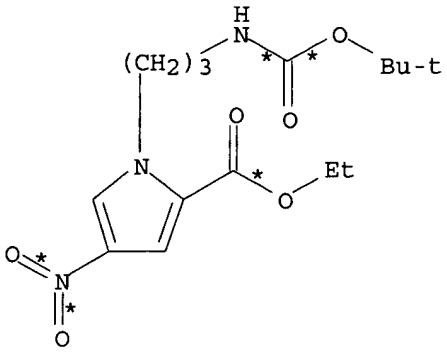
ACCESSION NUMBER: 139:365206 CASREACT
TITLE: Solid-phase synthesis of core 2 O-linked glycopeptide and its enzymatic sialylation
AUTHOR(S): Takano, Yutaka; Kojima, Naoya; Nakahara, Yuko; Hojo, Hironobu; Nakahara, Yoshiaki
CORPORATE SOURCE: Institute of Glycotechnology, Department of Applied Biochemistry, Tokai University, Hiratsuka-shi, Kanagawa, 259-1292, Japan
SOURCE: Tetrahedron (2003), 59(42), 8415-8427
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The core 2-type tetrasaccharide building blocks I (R = H, Me; R1 = Fmoc; R2 = OH) for solid-phase synthesis of glycopeptide were synthesized via stereoselective glycosylation of the disaccharyl Ser/Thr II (All = allyl) with a glycosyl fluoride III carrying the 2-trichloroacetamido group that was readily converted into a 2-acetamido group by reduction Using building block I (R = Me, R1 = Fmoc, R2 = OH), a segment of glycoprotein leukosialin(215-224) I (R = Me, R1 = Fmoc-Pro-, R2 = -Thr-Ser-Thr-Asn-Ala-Ser-Thr-Val-NH2) was synthesized by the solid-phase protocol. Cleavage of the synthetic glycopeptide from resin was accomplished with reagent K and subsequent treatment of the product with a cocktail for the "low-acidity TfOH" facilitated complete removal of the benzyl groups with min. loss of glycosidic linkages. To the above glycopeptide, following Fmoc deprotection, N-acetylneuraminic acid (sialic acid) residues were enzymically introduced in remarkably high efficiency by using the specific sialyltransferases.
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

RX(10) OF 10 COMPOSED OF RX(1), RX(2), RX(3), RX(4)
RX(10) A + B + P + R + S + T + U + V ===> W



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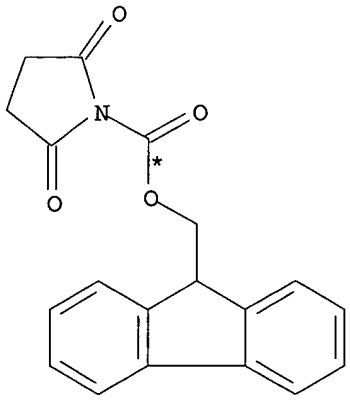

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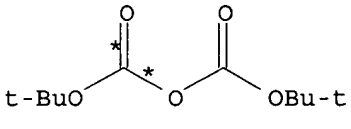

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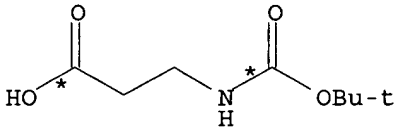

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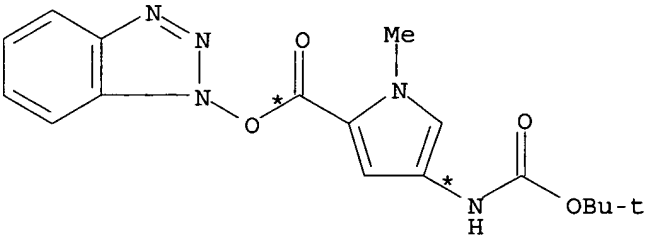

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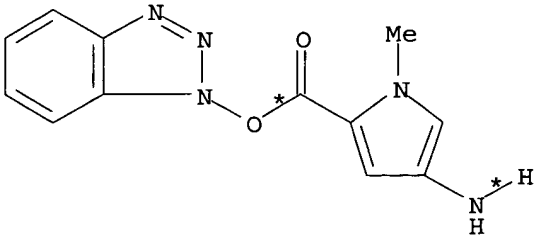

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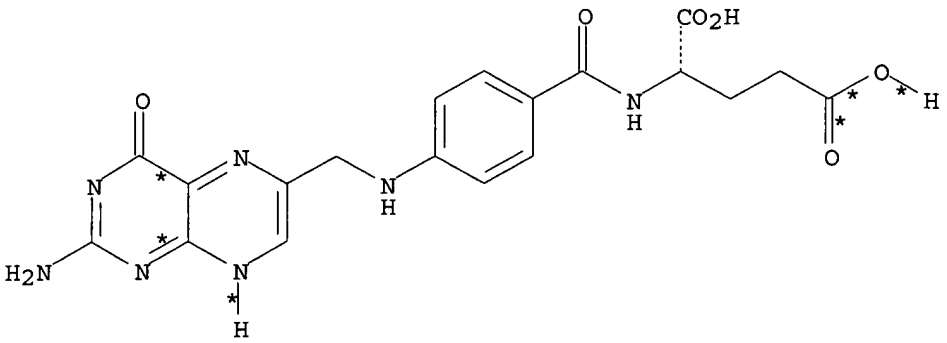

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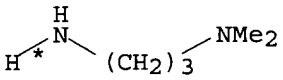
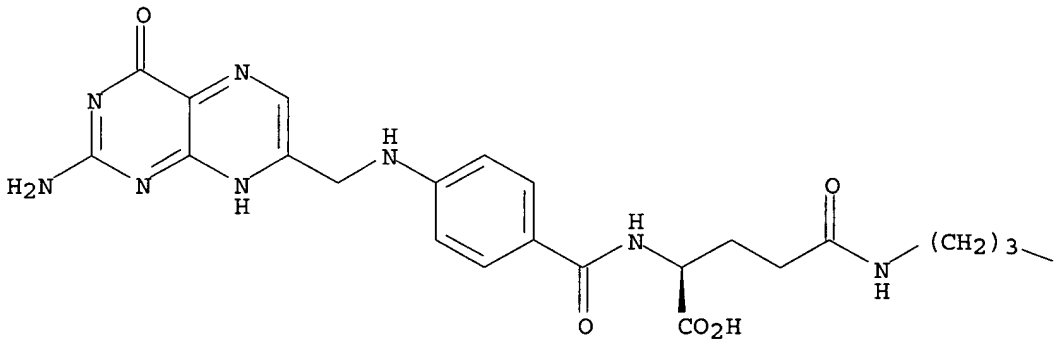


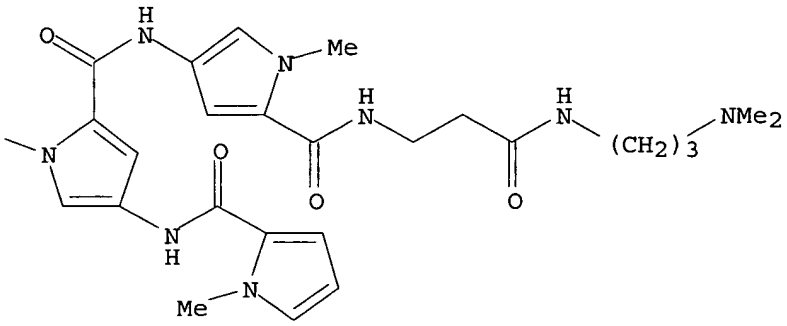
V

4
STEPS

PAGE 1-A



PAGE 1-B



W
YIELD 60%

RX(1) RCT A 159539-42-1

STAGE(1)
RGT D 1310-73-2 NaOH
SOL 7732-18-5 Water, 64-17-5 EtOH

STAGE(2)
RGT E 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(3)
RGT F 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2
CON 2 hours, 0 deg C -> room temperature

STAGE(4)
RCT B 102774-86-7
RGT G 497-19-8 Na2CO3
SOL 67-64-1 Me2CO, 7732-18-5 Water
CON 12 hours

PRO C 481070-51-3

RX(2) RCT C 481070-51-3
RGT M 1333-74-0 H2
PRO L 481070-49-9
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 2 hours

RX(3) RCT L 481070-49-9, P 24424-99-5
PRO Q 481070-50-2
SOL 67-56-1 MeOH
CON 2 hours, room temperature

RX(4) RCT R 3303-84-2D

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STAGE(1)
RGT F 76-05-1 F3CCO2H, X 108-98-5 PhSH
SOL 75-09-2 CH2Cl2

STAGE(2)
RCT S 77716-16-6
RGT Y 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 90 minutes

STAGE(3)
RGT F 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2

STAGE(4)
RCT Q 481070-50-2
RGT Z 2592-95-2 1-Benzotriazolol, AA 538-75-0 DCC, Y 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 90 minutes

STAGE(5)
RGT F 76-05-1 F3CCO2H, X 108-98-5 PhSH
SOL 75-09-2 CH2Cl2

STAGE(6)
RCT T 481070-52-4
RGT Y 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON 90 minutes

STAGE(7)
RCT U 59-30-3
RGT AB **110-89-4** Piperidine, AC **872-50-4** NMEP, AA 538-75-0 DCC, Z 2592-95-2 1-Benzotriazolol, Y 7087-68-5 EtN(Pr-i)2
CON 5 hours

STAGE(8)
RCT V 109-55-7
CON 5 hours, 55 deg C

PRO W 481070-53-5
NTE solid-state reaction, first stage attachment to Boc-β-alanine-Pam resin

ACCESSION NUMBER: 138:73505 CASREACT
TITLE: Solid-phase synthesis of a folate conjugate of a DNA binding polyamide
AUTHOR(S): Sharma, Sanjay K.; Lown, J. William
CORPORATE SOURCE: Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Can.
SOURCE: Tetrahedron Letters (2002), 43(37), 6665-6667
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Solid-phase synthesis of a folate tripyrrolocarboxamide conjugate of a DNA binding polyamide (I) by connecting N-methyloligopyrrolepolyamide to folic acid using new monomer (II) is described. The synthesis of a new building block monomer Boc-Py-[(CH2)3-NHFmoc] (Boc = tert-butoxycarbonyl, Fmoc = 9-fluorenylmethoxycarbonyl, Py = pyrrolidine) acid II is also reported.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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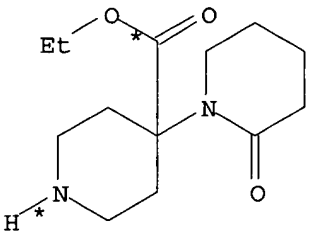
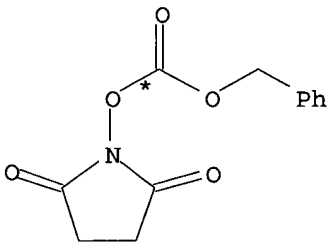
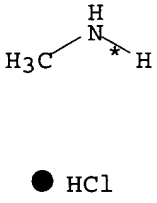
RX(354) OF 425 COMPOSED OF RX(24), RX(25), RX(26), RX(17), RX(50)
RX(354) **CE** + CF + CI + B + K ===> EI



CE



CF



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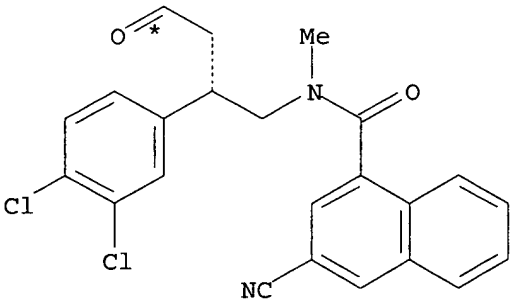

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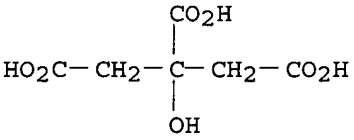
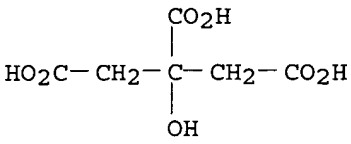
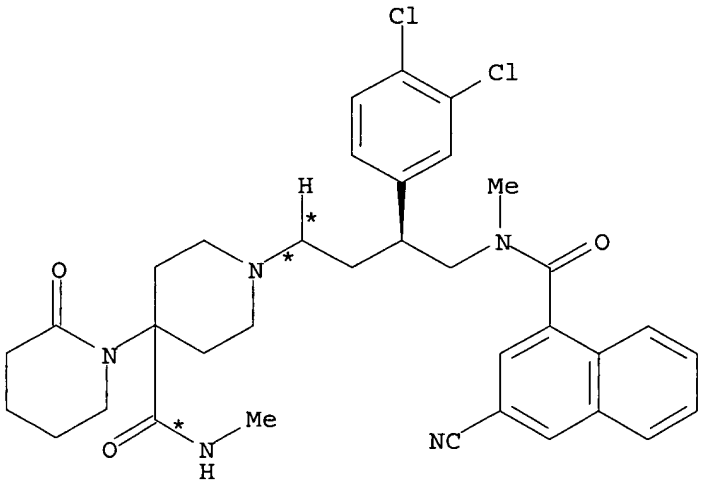


K

5 STEPS



EI: CM 1



EI: CM 2

RX(24) RCT CE **166180-90-1**, CF 13139-17-8
RGT BG 121-44-8 Et3N
PRO CG 166180-93-4
SOL 75-09-2 CH2Cl2

RX(25) RCT CG 166180-93-4
RGT BA 1310-73-2 NaOH
PRO CH 166180-94-5
SOL 109-99-9 THF, 7732-18-5 Water

RX(26) RCT CH 166180-94-5, CI 593-51-1
RGT CJ 465535-95-9 1,3-Propanediamine, N'-carbonimidoyl-N,N-dimethyl-, monohydrochloride, CK 1122-58-3 4-DMAP
PRO BP 166181-27-7
SOL 75-09-2 CH2Cl2

RX(17) RCT BP 166181-27-7
RGT BQ 1333-74-0 H2
PRO O 166181-38-0
CAT 63310-18-9 Pd hydroxide
SOL 64-17-5 EtOH
NTE catalyst on carbon

RX(50) RCT B 255050-50-1, O 166181-38-0

STAGE(1)
SOL 67-56-1 MeOH

STAGE(2)
RGT E 64-19-7 AcOH

STAGE(3)
RGT F 25895-60-7 NaBH3CN

STAGE(4)
RGT R 144-55-8 NaHCO3
SOL 7732-18-5 Water

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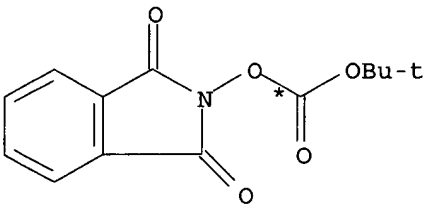
STAGE(5)
RCT K 77-92-9

PRO EI 255049-93-5

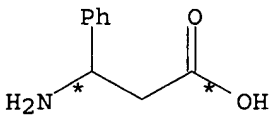
ACCESSION NUMBER: 137:272794 CASREACT
TITLE: Design, Synthesis, and SAR of Tachykinin Antagonists: Modulation of Balance in NK1/NK2 Receptor Antagonist Activity
AUTHOR(S): Albert, Jeffrey S.; Aharony, David; Andisik, Donald; Barthlow, Herbert; Bernstein, Peter R.; Bialecki, Russell A.; Dedinas, Robert; Dembofsky, Bruce T.; Hill, Daniel; Kirkland, Karin; Koether, Gerard M.; Kosmider, Benedict J.; Ohnmacht, Cyrus; Palmer, William; Potts, William; Rumsey, William; Shen, Lihong; Shenvi, Ashok; Sherwood, Scott; Warwick, Paul J.; Russell, Keith
CORPORATE SOURCE: CNS Discovery Research, AstraZeneca Pharmaceuticals LP, Wilmington, DE, 19850-5437, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(18), 3972-3983
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Through optimization of compds. based on the dual NK1/NK2 antagonist ZD6021, it was found that alteration of two key regions could modulate the balance of NK1 and NK2 potency. Substitution of the 2-naphthalene position in analogs of ZD6021 resulted in increased NK1 potency and thus afforded NK1 preferential antagonists. Alterations of the piperidine region could then increase NK2 potency to restore dual NK1/NK2 selectivity. Through these efforts, three novel receptor antagonists from a single chemical related series were identified; two are dual NK1/NK2 antagonists, and the third is an NK1 preferential antagonist. In this paper, the factors affecting the balance of NK1 and NK2 selectivity in this series are discussed and the in vitro and in vivo properties of the novel antagonists are described.
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

RX(42) OF 199 COMPOSED OF REACTION SEQUENCE RX(9), RX(8)
AND REACTION SEQUENCE RX(6), RX(7), RX(8)
...AH + AI ===> AC...
... **U** + AC ===> **AD**



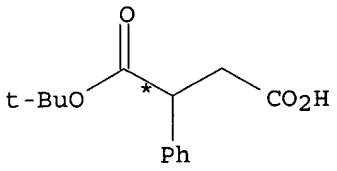
AH



AI

3 STEPS

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86



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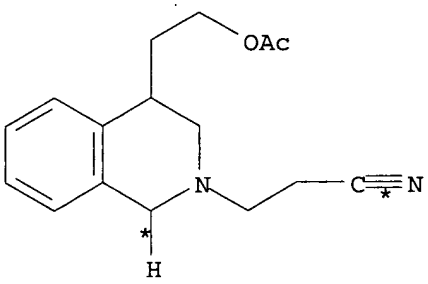

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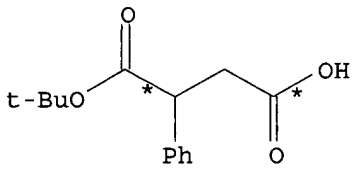
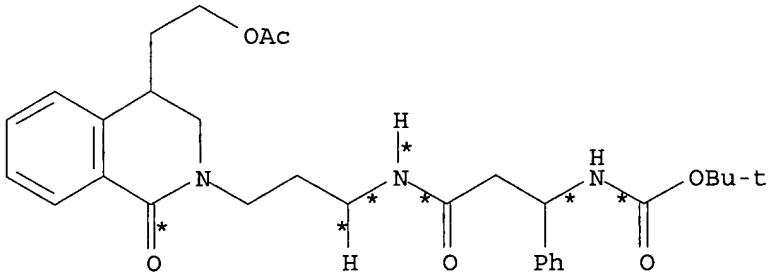


AC

3 STEPS



AD

RX(9) RCT AH 15263-20-4, AI 614-19-7
PRO AC 104465-81-8
SOL 68-12-2 DMF, 7732-18-5 Water

RX(6) RCT U **104465-78-3**
RGT W 7722-64-7 KMnO4, X 7487-88-9 MgSO4
PRO V 104465-79-4
SOL 67-64-1 Me2CO, 7732-18-5 Water

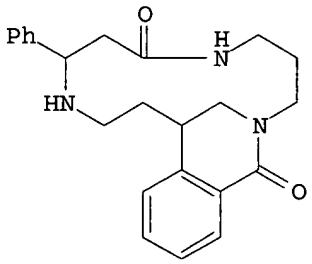
RX(7) RCT V 104465-79-4
RGT L 1333-74-0 H2
PRO Z 104465-80-7
CAT 11129-89-8 Pt oxide
SOL 67-66-3 CHCl3, 64-17-5 EtOH

RX(8) RCT AC 104465-81-8, Z 104465-80-7
RGT AE 14338-32-0 2-Cl-py.MeI, AF 121-44-8 Et3N

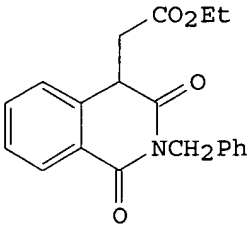
Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

PRO AD **104465-82-9**
SOL 75-09-2 CH2Cl2

ACCESSION NUMBER: 106:5298 CASREACT
TITLE: Total synthesis of ±-isocyclocelabenzene
AUTHOR(S): Iida, Hideo; Fukuhara, Kiyoshi; Murayama, Yoshiaki; Machiba, Mitsuo; Kikuchi, Toyohiko
CORPORATE SOURCE: Tokyo Coll. Pharm., Horinouchi Hachioji, 192-03, Japan
SOURCE: Journal of Organic Chemistry (1986), 51(24), 4701-3
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB The macrocyclic spermidine alkaloid isocyclocelabenzene (I) was synthesized from homophthalimide derivative II and 3-amino-3-phenylpropionic acid.

=> fil caplus;s werpy t?/au

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	159.59	303.10

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.97	-10.65

FILE 'CAPLUS' ENTERED AT 16:23:27 ON 31 JAN 2006

FILE COVERS 1907 - 31 Jan 2006 VOL 144 ISS 6

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

FILE LAST UPDATED: 30 Jan 2006 (20060130/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

L12 28 WERPY T?/AU

=> s frye j?/au;s white j?/au;s zacher a?/au
L13 263 FRYE J?/AU

L14 8093 WHITE J?/AU

L15 20 ZACHER A?/AU

=> s l12 and l13 and l14 and l15
L16 1 L12 AND L13 AND L14 AND L15

=> d ibib abs

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:566590 CAPLUS
DOCUMENT NUMBER: 141:123556
TITLE: Process for producing N-methylsuccinimide from dicarbonyl compounds by cyclization and alkylation and hydrogenation to N-methylpyrrolidinone
INVENTOR(S): **Werpy, Todd A.**; **Frye, John G., Jr.**; **White, James F.**; Holladay, Johnathan E.; **Zacher, Alan H.**
PATENT ASSIGNEE(S): Battelle Memorial Institute, USA
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

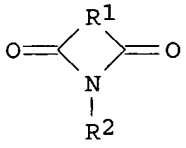
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004058708	A1	20040715	WO 2003-US40106	20031216
WO 2004058708	B1	20040923		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004176589	A1	20040909	US 2003-731108	20031210
EP 1572644	A1	20050914	EP 2003-814062	20031216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.: US 2002-435469P P 20021220

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

	US 2003-108336	A	20031210
	US 2003-731108	A	20031210
	WO 2003-US40106	W	20031216

OTHER SOURCE(S): CASREACT 141:123556; MARPAT 141:123556
GI



I

AB The invention includes methods of processing an initial di-carbonyl compound by conversion to a cyclic compound I (R1 = linear or branched, saturated or unsatd. hydrocarbon or substituted hydrocarbon; R2 = H; linear, cyclic or branched, saturated or unsatd. alkyl; aromatic group). The cyclic compound is reacted with an alkylating agent to form a derivative having an alkylated ring nitrogen. The invention encompasses a method of producing an N-alkyl product. Ammonia content of a solution is adjusted to produce a ratio of ammonia to dicarboxylate compound of from about 1:1 to about 1.5:1. An alkylating agent is added and the initial compound is alkylated and cyclized. The invention includes methods of making N-methylpyrrolidinone (NMP). Aqueous ammonia and succinate is introduced into a vessel and ammonia is adjusted to provide a ratio of ammonia to succinate of less than 2:1. A methylating agent is reacted with succinate at a temperature of from greater than 100° to about 400° to produce N-methylsuccinimide which is purified and hydrogenated to form NMP.

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=> s (l12 or l13 or l14 or l15) and ?succinimide?
         30895 ?SUCCINIMIDE?
L17          7 (L12 OR L13 OR L14 OR L15) AND ?SUCCINIMIDE?

=> d 1-7 ibib abs hitstr
```

L17 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:566590 CAPLUS
DOCUMENT NUMBER: 141:123556
TITLE: Process for producing N-**methylsuccinimide** from dicarbonyl compounds by cyclization and alkylation and hydrogenation to N-methylpyrrolidinone
INVENTOR(S): **Werpy, Todd A.**; **Frye, John G., Jr.**; **White, James F.**; Holladay, Johnathan E.; **Zacher, Alan H.**
PATENT ASSIGNEE(S): Battelle Memorial Institute, USA
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004058708	A1	20040715	WO 2003-US40106	20031216

WO 2004058708 B1 20040923
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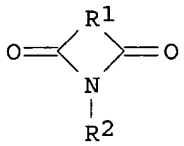
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
US 2004176589 A1 20040909 US 2003-731108 20031210
EP 1572644 A1 20050914 EP 2003-814062 20031216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
PRIORITY APPLN. INFO.: US 2002-435469P P 20021220
US 2003-108336 A 20031210
US 2003-731108 A 20031210
WO 2003-US40106 W 20031216
OTHER SOURCE(S): CASREACT 141:123556; MARPAT 141:123556
GI



I

AB The invention includes methods of processing an initial di-carbonyl compound by conversion to a cyclic compound I (R1 = linear or branched, saturated or unsatd. hydrocarbon or substituted hydrocarbon; R2 = H; linear, cyclic or branched, saturated or unsatd. alkyl; aromatic group). The cyclic compound is reacted with an alkylating agent to form a derivative having an alkylated ring nitrogen. The invention encompasses a method of producing an N-alkyl product. Ammonia content of a solution is adjusted to produce a ratio of ammonia to dicarboxylate compound of from about 1:1 to about 1.5:1. An alkylating agent is added and the initial compound is alkylated and cyclized. The invention includes methods of making N-methylpyrrolidinone (NMP). Aqueous ammonia and succinate is introduced into a vessel and ammonia is adjusted to provide a ratio of ammonia to succinate of less than 2:1. A methylating agent is reacted with succinate at a temperature of from greater than 100° to about 400° to produce N-**methylsuccinimide** which is purified and hydrogenated to form NMP.

L17 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:977786 CAPLUS
DOCUMENT NUMBER: 138:57825
TITLE: Method and catalysts of making pyrrolidones by hydrogenation
INVENTOR(S): **Werpy, Todd**; **Frye, John G., Jr.**; Wang, Yong; **Zacher, Alan H.**
PATENT ASSIGNEE(S): Battelle Memorial Institute, USA
SOURCE: PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002102772	A1	20021227	WO 2002-US19372	20020617
WO 2002102772	B1	20031120		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003097006	A1	20030522	US 2001-884602	20010618
US 6603021	B2	20030805		
EP 1412329	A1	20040428	EP 2002-756233	20020617
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003114687	A1	20030619	US 2002-280577	20021025
US 6706893	B2	20040316		
US 2003120087	A1	20030626	US 2002-280462	20021025
US 6670483	B2	20031230		
US 2003125570	A1	20030703	US 2002-280622	20021025
US 6632951	B2	20031014		

PRIORITY APPLN. INFO.: US 2001-884602 A 20010618
WO 2002-US19372 W 20020617

OTHER SOURCE(S): MARPAT 138:57825

AB The present invention provides methods for making N-methylpyrrolidine and analogous compds. via hydrogenation. Catalysts for this process comprise carbon, metal oxides, and Pd, Rh, PT, Ru, Ni, and/or Co. Other process improvements may include extraction and hydrolysis steps. Some preferred reactions take place in the aqueous phase. Starting materials for making N-methylpyrrolidine may include succinic acid, N-**methylsuccinimide**, and their analogs.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:962011 CAPLUS
DOCUMENT NUMBER: 138:154086
TITLE: Neutron and X-ray Reflectivity from Polyisobutylene-Based Amphiphiles at the Air-Water Interface
AUTHOR(S): Reynolds, Philip A.; McGillivray, Duncan J.; Gilbert, Elliot P.; Holt, Stephen A.; Henderson, Mark J.; **White, John W.**
CORPORATE SOURCE: Research School of Chemistry, The Australian National University, Canberra, 0200, Australia
SOURCE: Langmuir (2003), 19(3), 752-761
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have performed X-ray and neutron reflectivity expts. on amphiphile films spread at the air-water and air-saturated ammonium nitrate solution

interfaces as a function of film compression. We have examined ca. 750, 1100, and 1700 mol. weight monodisperse polyisobutylene amide (PIBSA), 1100 imide (PIBSIM), and also palmitic acid for the pure amphiphiles and binary mixts. We have used deuterated and hydrogenous components so that a given film may be examined in up to seven contrasts. All of the films form a monolayer, with mol. area determined by tail group size, which increases slightly in thickness on compression for PIB derivs. There are differences in film thicknesses as shown by a dependence on compression and substructure; this is understood in terms of the increasing tendency of the tail to adopt a coiled conformation as mol. weight increases. PIBSA films consist of packed micrometer scale disks containing up to 10% open water (polynya) area. Palmitic acid-containing films contain a greater polynya area. All films lose up to half of the original amount of amphiphile from the monolayer when compressed. The almost reversible loss of material followed the trend palmitic acid < 750 amide < 1100 amide < 1100 imide, empirically in order of hydrophile-lipophile balance (HLB) number This pattern suggests an amphiphile loss into submicrometer aggregates at the interface, rather than dispersion into the aqueous phase. Binary mixts. exhibit differential competition of the components to remain in the monolayer with the trend: palmitic acid >750 amide > 1100 amide > 1100 imide, opposite to the aggregation tendency as expected. The preference to remain at the surface may be phys. related to more effective packing of the headgroup mols. on the surface when head and tail areas are better matched in size. Mixts. also spontaneously segregate laterally and form micrometer scale domains. This tendency also follows the HLB number, with better mixing for those components with similar HLB values. Lateral segregation is encouraged by film compression. Surprisingly, properties of films on water and 50 wt% ammonium nitrate subphase show little difference with respect to these trends.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:541397 CAPLUS

DOCUMENT NUMBER: 135:344623

TITLE: Asymmetric synthesis of (+)-loline, a pyrrolizidine alkaloid from rye grass and tall fescue

AUTHOR(S): Blakemore, Paul R.; Kim, Sung-Kee; Schulze, Volker K.; **White, James D.**; Yokochi, Alexandre F. T.

CORPORATE SOURCE: Department of Chemistry, Oregon State University, Corvallis, OR, 97331-4003, USA

SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2001), (15), 1831-1847
CODEN: JCSPCE; ISSN: 1472-7781

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:344623

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB (+)-Loline (I) was synthesized via a pathway that employed intramol. [4 + 2] cycloaddn. of an acylnitrosodiene, (S,E)-H2C:CHCH:CHCH(OR1)CH2CON:O (R1 = SiMe2CMe3, CH2C6H4OMe-4), as a key step. The acylnitrosodienes, which were used in situ, were obtained by oxidation of the corresponding hydroxamic acids, (S,E)-H2C:CHCH:CHCH(OR2)CH2CONHOH (R2 = SiMe2CMe3, CH2C6H4OMe-4),

and these were prepared from either glucose via aldehyde II or more directly from (S)-malic acid. The endo dihydrooxazines III (R3 = SiMe2CMe3, CH2C6H4OMe-4), obtained in a mixture with their exo stereoisomer, were transformed by reductive N-O bond cleavage and reannulation into pyrrolizines IV (R4 = SiMe2CMe3, CH2C6H4OMe-4). The latter was subjected to Sharpless aminohydroxylation in the presence of (DHQD)2PHAL to give V (R5 = R6 = H) along with its regioisomer. N-Methylation of tosyl amide V (R5 = R6 = H), followed by mesylation of alc. V (R5 = H; R6 = Me) and reduction of the γ-lactam V (R5 = SO2Me; R6 = Me) with borane, afforded pyrrolizidine VI (R7 = CH2C6H4OMe-4). Cleavage of the p-methoxybenzyl ether and subsequent thermal treatment of VI (R7 = H) resulted in intramol. etherification to yield N-tosylloline (VII). Final reductive cleavage of the N-tosyl residue produced (+)-loline (I), characterized as its dihydrochloride.

REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:441402 CAPLUS
DOCUMENT NUMBER: 107:41402
TITLE: Synthesis of a new thermally curable elastomer via regioselective chlorination of a polyimidosulfide
AUTHOR(S): **White, Jerry E.**
CORPORATE SOURCE: Cent. Res.-Polym. Mater. Lab., Dow Chem. Co., Midland, MI, 48674, USA
SOURCE: Journal of Polymer Science, Part A: Polymer Chemistry (1987), 25(4), 1191-5
CODEN: JPACEC; ISSN: 0887-624X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The title rubber was synthesized from the reaction of N-**chlorosuccinimide** with a polyimidosulfide which was prepared by polymerization of 1,4-butanediol and N,N'-bismaleimido-1,8-octane. NMR spectrum showed a vinyl proton absorption at δ = 5.90 whose integration along with integrations of ring CH and CH2 protons were consistent with the composition

L17 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:406776 CAPLUS
DOCUMENT NUMBER: 103:6776
TITLE: Step-growth polymers from bismaleimides. Synthesis and reactions of some new polyimides
AUTHOR(S): **White, Jerry E.**; Scaia, Mark D.; Snider-Tung, Deborah A.
CORPORATE SOURCE: Cent. Res., Dow Chem. Co., Midland, MI, 48640, USA
SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1985), 26(1), 132-3
CODEN: ACPPAY; ISSN: 0032-3934
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Linear high-mol.-weight polyaspartimide were prepared in 58-84% yield by poly addition of N,N'-dimethyl-1,6-hexanediamine or piperazine with bismaleimides. Polyimidosulfides in 75-86% yield were prepared by addition of dithiols with bismaleimides.

L17 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:48570 CAPLUS
DOCUMENT NUMBER: 102:48570
TITLE: Soluble oil cutting fluid

INVENTOR(S): Rawlinson, Anthony Paul; **White, James**
PATENT ASSIGNEE(S): British Petroleum Co. PLC, UK
SOURCE: Eur. Pat. Appl., 11 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 120665	A2	19841003	EP 1984-301863		19840320
EP 120665	A3	19850403			
EP 120665	B1	19870513			
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE					
AU 8425867	A1	19840927	AU 1984-25867		19840319
AU 558608	B2	19870205			
AT 27174	E	19870515	AT 1984-301863		19840320
CA 1223243	A1	19870623	CA 1984-450069		19840321
DK 8401632	A	19840924	DK 1984-1632		19840322
ZA 8402146	A	19851127	ZA 1984-2146		19840322
PRIORITY APPLN. INFO.:			GB 1983-7975	A	19830323
			EP 1984-301863	A	19840320

AB A soluble-oil concentrate, to be diluted with H2O, comprises an alkali or alkaline-earth alkylbenzenesulfonate, a fatty acid diethanolamide, a mixed alkanolamine borate, a polyisobutene derivative of **succinimide**, and mineral oil. The soluble oil is stable without containing a conventional coupling agent; some soluble-oil emulsions are biostatic, even though conventional biocides are not included.

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(FILE 'HOME' ENTERED AT 16:10:59 ON 31 JAN 2006)

FILE 'CASREACT' ENTERED AT 16:11:08 ON 31 JAN 2006
L1 STR
L2 STR L1
L3 0 S L2
L4 2 S L2 FUL
L5 6 S WERPY ?/AU

FILE 'CASREACT' ENTERED AT 16:20:25 ON 31 JAN 2006
L6 STR L3
L7 50 S L6
L8 2816 S L6 FUL
L9 STR L2
L10 9 SEARCH L9 SUB=L8 FUL
L11 7 S L10 NOT L4

FILE 'CAPLUS' ENTERED AT 16:23:27 ON 31 JAN 2006
L12 28 S WERPY T?/AU
L13 263 S FRYE J?/AU
L14 8093 S WHITE J?/AU
L15 20 S ZACHER A?/AU
L16 1 S L12 AND L13 AND L14 AND L15
L17 7 S (L12 OR L13 OR L14 OR L15) AND ?SUCCINIMIDE?

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

```
=> fil reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                        33.97     337.07

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)              SINCE FILE      TOTAL
                                                           ENTRY    SESSION
CA SUBSCRIBER PRICE                                        -6.00     -16.65

FILE 'REGISTRY' ENTERED AT 16:26:43 ON 31 JAN 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   30 JAN 2006  HIGHEST RN 873057-98-8
DICTIONARY FILE UPDATES:  30 JAN 2006  HIGHEST RN 873057-98-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                    *
**********************************************************************

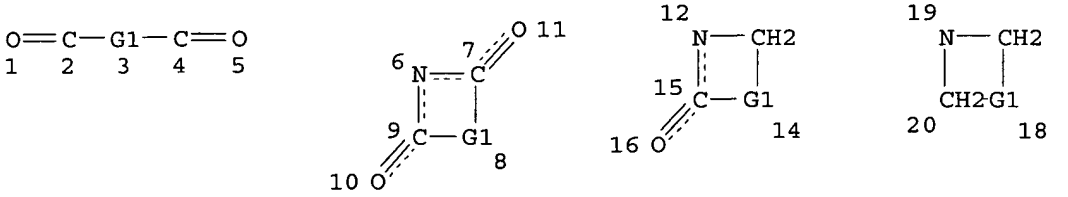
Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> e "n-methyl succinimide"/cn 5
E1            1     N-METHYL PHOSPHOROAMIDODICHLORIDATE/CN
E2            1     N-METHYL PROSCILLARIDIN A LACTAM/CN
E3            0 --> N-METHYL SUCCINIMIDE/CN
E4            1     N-METHYL TAXOL A/CN
E5            1     N-METHYL TETRAFLUOROPHTHALIMIDE/CN

=> d l4 que stat
L2              STR
```



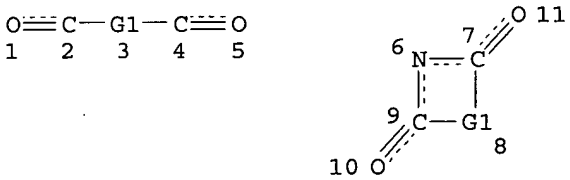
REP G1=(2-4) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L4 2 SEA FILE=CASREACT SSS FUL L2 (42 REACTIONS)

100.0% DONE 73794 VERIFIED 42 HIT RXNS 2 DOCS
SEARCH TIME: 00.00.07

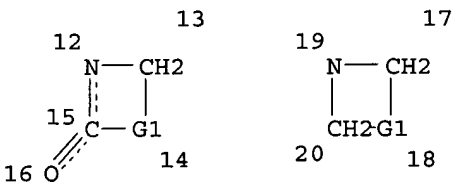
=> d l10 que stat
L6 STR



REP G1=(2-4) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L8 2816 SEA FILE=CASREACT SSS FUL L6 (52585 REACTIONS)
L9 STR



REP G1=(2-4) C

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

```
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   9

STEREO ATTRIBUTES: NONE
L10           9 SEA FILE=CASREACT SUB=L8 SSS FUL L9 (   124 REACTIONS)

100.0% DONE   51070 VERIFIED     124 HIT RXNS                      9 DOCS
SEARCH TIME: 00.00.01


=> dis his

     (FILE 'HOME' ENTERED AT 16:10:59 ON 31 JAN 2006)

     FILE 'CASREACT' ENTERED AT 16:11:08 ON 31 JAN 2006
L1              STR
L2              STR L1
L3            0 S L2
L4            2 S L2 FUL
L5            6 S WERPY ?/AU

     FILE 'CASREACT' ENTERED AT 16:20:25 ON 31 JAN 2006
L6              STR L3
L7           50 S L6
L8         2816 S L6 FUL
L9              STR L2
L10           9 SEARCH L9  SUB=L8 FUL
L11           7 S L10 NOT L4

     FILE 'CAPLUS' ENTERED AT 16:23:27 ON 31 JAN 2006
L12          28 S WERPY T?/AU
L13         263 S FRYE J?/AU
L14        8093 S WHITE J?/AU
L15          20 S ZACHER A?/AU
L16           1 S L12 AND L13 AND L14 AND L15
L17           7 S (L12 OR L13 OR L14 OR L15) AND ?SUCCINIMIDE?

     FILE 'REGISTRY' ENTERED AT 16:26:43 ON 31 JAN 2006
               E "N-METHYL SUCCINIMIDE"/CN 5

=> log y
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                  ENTRY    SESSION
FULL ESTIMATED COST                                0.44     337.51

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                  ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00     -16.65

STN INTERNATIONAL LOGOFF AT 16:27:24 ON 31 JAN 2006
```